

Supplemental Information for:

**Effects of Cations on Protein and Peptide Charging in Electrospray Ionization from  
Aqueous Solutions**

Anna C. Susa, Daniel N. Mortensen and Evan R. Williams\*

*Department of Chemistry, University of California, Berkeley, California 94720-1460*

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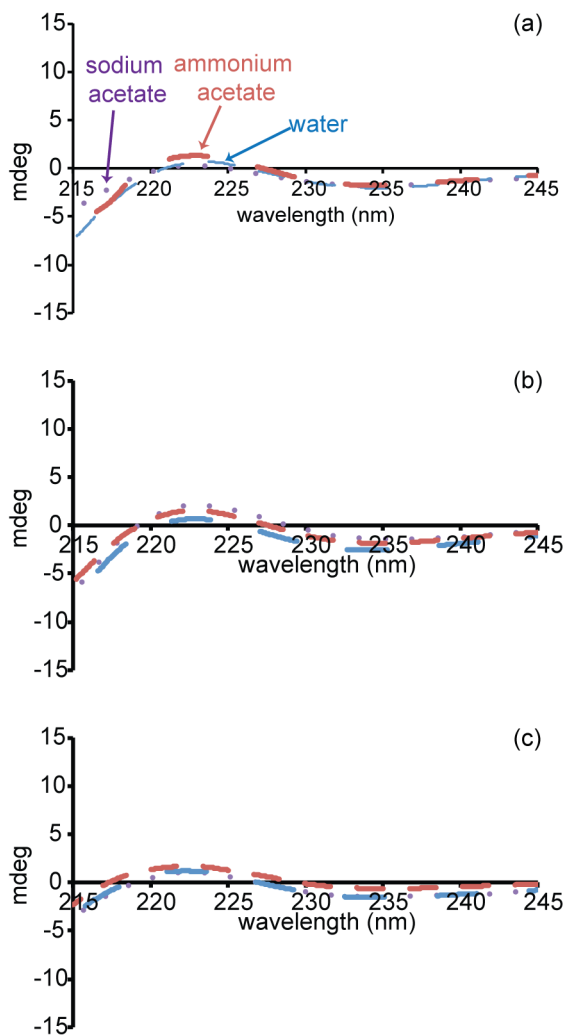
\*Address correspondence to Prof. Evan R. Williams:

Department of Chemistry  
University of California, Berkeley  
B42 Hildebrand Hall Berkeley, CA 94720  
Phone: (510) 643-7161  
e-mail: [erw@berkeley.edu](mailto:erw@berkeley.edu)

## Supplemental Table 1

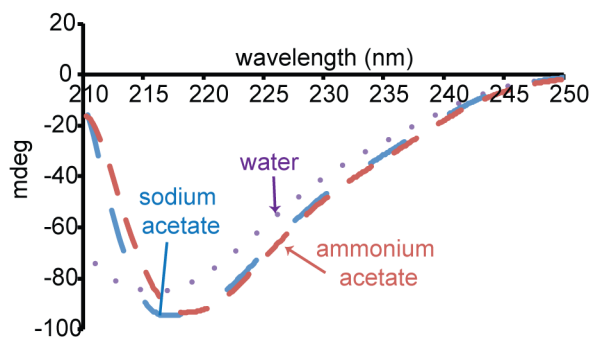
Average number of cation adducts per charge state of each protein/peptide ion.

<i>protein/peptide</i>	<i>Charge state</i>	<i>Average number of adducts</i>							
		<i>Li<sup>+</sup></i>	<i>Na<sup>+</sup></i>	<i>K<sup>+</sup></i>	<i>Rb<sup>+</sup></i>	<i>NH<sub>4</sub><sup>+</sup></i>	<i>Cs<sup>+</sup></i>	<i>TMA<sup>+</sup></i>	<i>TEA<sup>+</sup></i>
<b>angiotensin II</b>	1+	0.7	0.7	0.7	1.3	0.0	1.0	2.3	2.0
	2+	4.0	4.0	4.3	4.0	0.0	2.7		0.3
<b>bradykinin</b>	1+	1.0	0.0	0.0	1.0	0.0	2.0	2.0	2.0
	2+	4.0	4.0	2.0	4.0	0.0	4.0	0.0	0.0
<b>SubP</b>	1+					0.0		1.0	1.0
	2+	1.7	2.0	1.7	2.0	0.0	2.0	0.0	0.0
	3+	1.0		1.0	0.0	0.0	0.0	0.0	0.0
<b>SubPOMe</b>	1+	0.3				0.0		1.0	1.0
	2+	2.0	3.0	3.0	2.0	0.0	3.0	0.0	0.0
	3+	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>SubPOH</b>	1+		0.0			0.0	0.0	2.0	2.0
	2+	3.0	3.0	3.0	3.0	0.0	2.7	0.0	0.0
	3+			0.0	0.0	0.0	0.0		
<b>ubiquitin</b>	2+								
	3+							12.0	5.7
	4+		0.7		0.3	0.0	0.7	28.0	11.7
	5+	5.8	26.7	14.7	9.0	0.0	10.3		
	6+	6.7	1.7	0.3		0.0			
<b>lysozyme</b>	3+								7.0
	4+							10.0	7.7
	5+							2.0	
	6+		1.0	5.3	3.0	0.0	3.0	0.0	
	7+	3.7	26.7	7.7	5.7	0.0	5.7		
	8+	1.0	9.3	4.7	4.7	0.0	2.0		
	9+	1.0	2.0	3.0	3.0	0.0	1.0		
	10+	0.0							
<b>β-lactoglobulin</b>	4+								3.0
	5+							9.0	6.7
	6+	0.3	20.1			0.0		12.0	
	7+	3.0	20.0	24.7	11.0	0.0	10.0		
	8+	5.0	36.7	35.1	9.7	0.0	5.5		
	9+	0.0				0.0	2.0		
	10+	0.0							



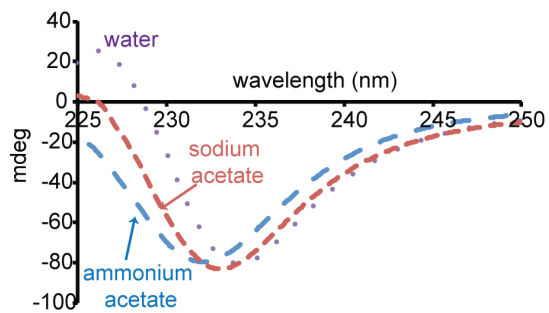
**Supplemental Figure 1**

CD spectra of 50  $\mu$ M (a) SubPOH, (b) SubPNH<sub>2</sub>, and (c) SubPOMe in water (blue dashed line), 25 mM sodium acetate (purple dotted line) and 25 mM ammonium acetate (red dashed line).



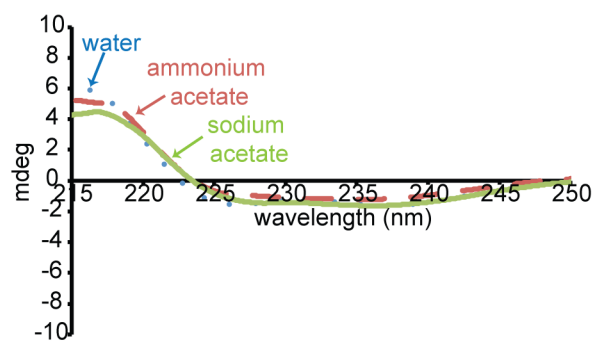
### Supplemental Figure 2

CD spectra of 25  $\mu$ M  $\beta$ -lactoglobulin in water (blue dashed line), 25 mM sodium acetate (purple dotted line) and 25 mM ammonium acetate (red dashed line).



### Supplemental Figure 3

CD spectra of 25  $\mu$ M lysozyme in water (purple dotted line), 25 mM sodium acetate (red dashed line) and 25 mM ammonium acetate (blue dashed line).



#### Supplemental Figure 4

CD spectra of 25  $\mu$ M angiotensin II in water (blue dotted line), 25 mM ammonium acetate (red dashed line) and 25 mM sodium acetate (green line).